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TECHNICAL DATA BULLETIN FOR DI-CUP (DICUMYL PEROXIDE) INCLUDING TOXICITY DATA FOR A-METHYLSTYRENE, ONE OF ITS DECOMPOSITION PRODUCTS		
Chemical Category		
A-METHYLSTYRENE (98-83-9)		

HERCULES

TECHNICAL DATA

DI-CUP PEROXIDE

BULLETIN ORC-204A
(Supersedes ORC-204)

86-870001667

α-Methylstyrene (p. 4)

DI-CUP® DICUMYL PEROXIDE DECOMPOSITION PRODUCTS –

SUMMARY OF TOXICOLOGICAL INVESTIGATIONS

The original bulletin on the subject (T-104) presented toxicological data on Di-Cup® dicumyl peroxide alone. However, in all of its uses as a peroxidic catalyst, its decomposition products (acetophenone, dimethylbenzyl alcohol, and *alpha*-methylstyrene) are also present. This bulletin, therefore, has been prepared to summarize the toxicological information obtained on all four compounds. These data are presented in detail on the following pages and also summarized in Table I, page 5.

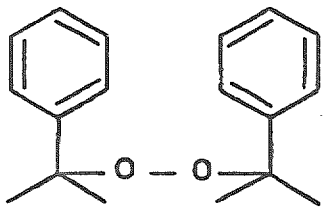
Summary

Di-Cup and its decomposition products are only slightly toxic by ingestion or inhalation. Mild eye and skin irritation may be encountered from accidental exposure to liquids or vapors.

The decomposition products of Di-Cup, however, are strong odorants. Low vapor concentrations result in persistent aromatic scents; when present in high concentrations, these odors may be objectionable.

Chemical Composition

Di-Cup is commercial dicumyl peroxide, available in three forms. The molecular weight of dicumyl peroxide is 270.36; its structural formula is shown below.



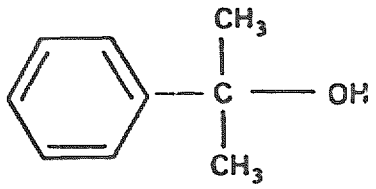
General Properties

The three forms of Di-Cup permit selection of the material most convenient for the application. Di-Cup 40C is a white, free-flowing powder that averages 40% active material supported on precipitated calcium carbonate. Di-Cup T, with an average of 90% dicumyl peroxide, is a pale yellow, low-melting, semicrystalline solid. Di-Cup R is a pale yellow to white, granular, low-melting crystalline solid, and is a more highly refined form that contains 95+% dicumyl peroxide. The

DIMETHYLBENZYL ALCOHOL (DMBA)

Chemical Composition

Dimethylbenzyl alcohol, molecular weight 136, has the following structural formula:



Acute Oral Toxicity

The oral LD_{50} in the rat ranged from 1,400 to 3,000 mg/kg. The oral LD_{50} in the rat of a mixture of 75% DMBA and 25% acetophenone was found to be 2000 mg/kg.

Eye Irritation

Application of 0.1 ml to the eyes of rabbits and 0.05 ml to the eyes of guinea pigs daily for 15 days produced some irritation with erythema. There was complete recovery within 7-14 days, with no permanent corneal damage.

Primary Irritation and Sensitization

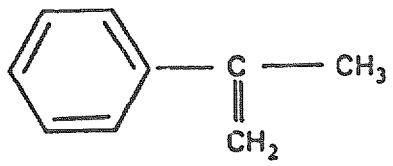
Guinea Pig and Rabbit Skin: Daily application of DMBA to the skin of rabbits and guinea pigs produced mild primary irritation.

Repeated Insult Patch Test: Fifty-five human subjects received 24-hr exposures to test patches three times weekly for 3 weeks and a challenge patch in the sixth week. There was little or no primary irritation. There was, however, a definite indication of skin sensitization in 7 of the 55 subjects, and more or less equivocal evidence of sensitization in 10 other subjects.

ALPHA-METHYLSTYRENE

Chemical Composition

Alpha-methylstyrene is a colorless liquid with a sharp, aromatic odor, a molecular weight of 118.15, and a boiling point of 165.4°C, and has the following structural formula:



Acute Oral Toxicity
The oral LD_{50} in the rat was found to be 4,800 mg/kg.

Eye Irritation
Application of two drops in the eyes of rabbits caused slight irritation of the conjunctiva, but no corneal damage.

Skin Irritation
Repeated applications to the skin of rabbits caused moderate to marked erythema. There was no indication of absorption with subsequent systemic toxic effects.

Acute Inhalation Toxicity
Vapor inhalation at 2,920 ppm (14 g/cu m) for 15-60 min caused respiratory irritation and central nervous system depression in rats, mice, and guinea pigs. Mice died after about 4 hrs, but rats and guinea pigs survived the 5-hr exposure.

Repeat Inhalation Toxicity
Exposure to 600 ppm produced minimum toxic effects to rabbits, rats, monkeys, and guinea pigs during 6-month inhalation study (7 hrs/day). No effects were detected at 200 ppm.

Methane, the simplest hydrocarbon, has no physiological action except when it lowers the partial pressure of oxygen in the air enough to cause effects due to oxygen deprivation. It has no warning odor.

Table I
TOXICITY SUMMARY
DI-CUP AND ITS DECOMPOSITION PRODUCTS

	Di-Cup	Acetophenone	DMBA	*alpha*-Methylstyrene
Acute oral toxicity (LD_{50}), mg/kg	4,100	900-3,000	1,400-3,000	4,700-4,900
Acute inhalation toxicity	90 mg/cu m—no effect	Saturated vapor—no deaths		14 g/cu m produced death (mice)
Eye irritation	Mild conjunctivitis	Irritation and transient corneal injury	Irritation with erythema	Irritation without corneal damage
Skin irritant (undiluted)	Mild irritation	Irritant	Mild irritation	Moderate irritation
Skin sensitizer	No	No	Yes	No

CERTIFICATE OF AUTHENTICITY

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